

## Preferential Solvation/Hydration of $\alpha$ -Chymotrypsin in Water-Acetonitrile Mixtures

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### Abstract

© 2017 American Chemical Society. The aim of our study is to monitor the preferential hydration/solvation of the protein macromolecules at low and high water content in water-organic mixtures. Our approach is based on the analysis of the absolute values of the water/organic solvent sorption. We applied this approach to estimate the protein stabilization/destabilization due to the preferential interactions of  $\alpha$ -chymotrypsin with water-acetonitrile mixtures. At high water content,  $\alpha$ -chymotrypsin is preferentially hydrated. At the intermediate water content, the preferential interaction changed from preferential hydration to preferential binding of acetonitrile. From infrared spectra, changes in the structure of  $\alpha$ -chymotrypsin were determined through an analysis of the structure of the amide I band. Acetonitrile augments the intensity of the 1626 cm<sup>-1</sup> band assigned to the intermolecular  $\beta$ -sheet aggregates. At low water content, the protein is in a glassy (rigid) state. The H-bond accepting acetonitrile molecules are not effective in solvating the dehydrated protein molecules alone. Therefore, the acetonitrile molecules are preferentially excluded from the protein surface, resulting in the preferential hydration. Advantages of our approach: (i) The preferential interaction parameters can be determined in the entire range of water content in water-organic mixtures. (ii) Our approach facilitates the individual evaluation of the Gibbs energies of water, protein, and organic solvent.

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